Effects of higher order excitations on the bandgap narrowing of quantum wires

A. Pahlavan¹, K. Nozari²,*

¹Department of Physics, Islamic Azad University, Sari Branch, Sari, Iran
²Departments of Physics, Faculty of Basic Sciences, University of Mazandaran, Babolsar, Iran

Received: 5 November 2009/Accepted: 12 February 2010/ Published: 20 June 2010

Abstract

The effects of higher order excitations on the bandgap renormalization of quasi-one dimensional semiconductor systems within the dynamical random phase approximation is studied. The contribution of the first and second excited states wave functions is incorporated in the calculation of the bandgap narrowing due to many-body exchange-correlation effects. It is shown that incorporation of the higher order excitations leads to the result that absolute values of the bandgap narrowing in these cases are larger than the corresponding renormalization which is calculated by only considering the ground state wave function.

PACS: 73.20.Dx; 71.35.Ee; 71.45.Gm

Keywords: Quantum wires; Many-body effects; Bandgap renormalization; Higher order excitations

1. Introduction

Optical pumping by intense laser beams can be used to generate a highly dense electron-hole plasma in a wide variety of semiconductor systems. The band structure and optical properties of highly excited semiconductors generally differ from those calculated for non-interacting electron-hole pairs due to many-body exchange-correlation effects in the electron-hole plasma [1,2]. In recent years, quasi-one dimensional semiconductor quantum wires have been fabricated in a variety of geometric shapes (such as rectangular, V-shaped, L-shaped, T-shaped and H-shaped) with atomic scale definition, and their optical properties have been studied for potential device applications such as semiconductor lasers [3-26]. The fundamental gap structure of these quasi-one dimensional systems changes due to the band gap renormalization (renormalization due to many-body exchange-correlation effects) when many-body effects are taken into account. This effect, as an important nonlinear optical effect in the semiconductor systems, has been studied for different geometries of the confinement potentials (see for instance [24-26] and references there in). Recently, the effect of external electric and magnetic fields on the bandgap renormalization of H-shaped quantum wires has been studied [26]. In this work our aim is to study the effects of higher order excitations on the band gap renormalization of the H-shaped quantum wires. By a suitable analytical definition of the quasi-one dimensional H-shaped confinement potential, we use a finite difference numerical scheme to calculate the eigenstates energies and wave functions of charge carriers in the presence of external electric and magnetic fields and for higher order excitations. This analysis will be performed within the Landau gauge for ground state and two first excited states. We obtain the profile of charge carriers distribution (probability amplitudes) in the presence of electric and magnetic fields for these states. As an important nonlinear optical property, the many-body exchange-correlation induced bandgap narrowing in this type of quantum wires is studied within the leading order dynamical random phase approximation. We focus mainly on the effects of higher order excitations on the values of the bandgap renormalization in this quasi-one dimensional system. A comparison between the results of different excitations will reveals the role played by higher order excitations in this low-dimensional system.

Fig. 1. The geometry of a typical H-Shaped quantum wire. Typical values of \( W_x \) and \( W_y \) are ~50-100 nm.

2. Theory

2.1. Mathematical simulation of the confinement potential

The geometry of a typical H-shaped quantum wire is shown in Fig. 1. This structure can be thought as two...
distinct T-shaped quantum wires joint together [26]. We consider the typical values of $W_x$ and $W_y$ to be of the order of 50-100 Nanometers. In order to account for the ballistic transport and the effect of confinement potential, we want to construct a possible model for a carrier in the two directions of confinement. Because of azimuthal symmetry, the Schrodinger equation is restricted to one dimension (the Schrodinger equation of the system is effectively two-dimensional but carriers are free to move in one dimension) where the confinement potential $V^{np}$ (the subscripts denote $n$ and $p$ type channel) can be simulated with the following analytical expression [26]:

$$
V(x,y) = \begin{cases} 
0 & \text{if} \quad -\infty < x < +\infty, \quad -\frac{3}{2}W_y \leq y \leq -W_y \\
-\infty < x < +\infty, \quad W_y \leq y \leq \frac{3}{2}W_y \\
-\frac{W_y}{2} \leq x \leq \frac{W_y}{2}, \quad -W_y \leq y \leq W_y \\
\infty & \text{elsewhere.}
\end{cases}
$$

We study many-body effects originated on the optical non-linearities in this quasi-one dimensional system in the presence of the external electric and magnetic fields.

2.2. Single particle states

In which follows, we study bound states and many-body effects in these quasi one dimensional systems in the presence of external electric and magnetic fields. The electric field is assumed to be directed along the $x$-axis and its typical value is of the order of a few $V/cm$. The presence of magnetic field is so that the Landau gauge, $\mathbf{A} = (0, Bx, 0)$ is satisfied. We first study the single particle properties in these quasi-one dimensional systems. The Hamiltonian of an electron in this configuration can be written as:

$$
H = \frac{1}{2m} \left[ p_x^2 + (p_y - eBx)^2 \right] - eEx
$$

where $e$ and $m$ are electron charge and mass, respectively. The Schrodinger equation of an electron with wave function $\Psi(x,y)$ can be written as:

$$
-\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \frac{2ieB}{\hbar} \frac{\partial}{\partial y} \right) \Psi(x,y)
+ \left( \frac{eB}{\hbar} \right)^2 x^2 \Psi(x,y)
- \frac{2meE}{\hbar^2} x \Psi(x,y) = \frac{2m}{\hbar^2} \lambda \Psi(x,y),
$$

where $\lambda$ stands for eigenvalues of energy, $E$ represents the magnitude of the electric field and $B$ is the magnitude of the magnetic field. To solve this eigenvalue problem we need to assign appropriate boundary conditions for each case. These boundary conditions are fixed by the external confinement potentials simulated with equation (1). It is necessary to emphasize that H-shaped geometry as shown in Fig.1 is the transverse section of the wire and that free carriers propagate in the direction normal to the plane of this figure. With definition of the confinement potential as (1) which provides also the required boundary conditions, we solve Eq. 3 numerically to find eigenvalues and eigenfunctions of an electron in the presence of the external electric and magnetic fields. Our numerical strategy is based on the finite difference algorithm and the results of these calculations for different external field configurations are shown in Figs. 2-6. In these figures, the asymmetry parameter which is defined as $\alpha \equiv W_x/W_y$ and measures relative width of the quantum wire in two directions of confinement in the plane of Fig. 1, has been set to be 0.8. We see that application of the external electric and magnetic fields leads to the break down of symmetry of charge carrier distribution relative to free-field case. In the absence of these fields, this distribution obeys the geometry of the confinement potential perfectly as Fig. 2 shows. The single-particle states wave functions obtained in this section will be used to study the bandgap renormalization of the H-shaped quantum wire in the next sections. For this purpose, first we give an overview of the theory of bandgap renormalization in quasi-one dimensional semiconductor systems.
the lowest exciton resonance. The exchange-correlation correction of the fundamental bandgap due to the presence of free carriers (electrons in the conduction band and holes in the valence band) in the system is referred to as the bandgap renormalization effect. Optical nonlinearities, which are strongly influenced by screening of the Coulomb interactions in the electron-hole plasma, are typically associated with the band gap re-normalization phenomenon. In which follows we use the two band (one conduction and one valance band) model to study the quasi-one dimensional electron-hole system. At the first step, we neglect the effects of higher subbands and degeneracies in valance bands. The effects of higher order excitations will be considered in the next section. For simplicity we assume that electrons and holes densities are constant in time. In this situation, Hamiltonian of the system can be written as (see Refs. [8,9,32]):

\[ H = H_1 + H_2, \]

where by definition:

\[ H_1 \equiv \frac{1}{2} \sum_k \left[ E_g^0 + \frac{k^2}{2m_e} c_k^\dagger c_k + \frac{k^2}{2m_h} d_k^\dagger d_k \right], \]

\[ H_2 \equiv \frac{1}{2L} \sum_{k,k',q} V_{c.e} e(q) c_{k+q}^\dagger c_k c_{k'}^\dagger c_{k+q} + V_{c.h} h(q) c_{k+q}^\dagger c_k c_{k'}^\dagger c_{k+q} + V_{c.e.h} e(q) c_{k+q}^\dagger c_k d_{k+q}^\dagger c_{k'} d_{k+q} \],

where \( c_k \) and \( c_k^\dagger \) are annihilation and creation operators for conduction band electrons, respectively. Also \( d_k \) and \( d_k^\dagger \) are annihilation and creation operators for valance band holes. \( E_g^0 \) is the direct band gap between the top of the valence band and the bottom of the conduction band. \( V_{c.e,h} \) show the possible three Coulomb interactions between electrons and holes. Note that two interactions in \( H_1 \) lead to electron-hole quasi particle self-energies, while \( H_2 \) leads to the production of excitonic bound states. Note also that this Hamiltonian consists of spin effects, although spin index is not included explicitly [8,9]. The Coulomb interaction matrix element in the one dimensional quantum wire is given by the following relation [8]:

\[ V_{c.e}(q) = \frac{e^2}{\pi} \int_{-\infty}^{+\infty} \, dx \, x' \int_{-\infty}^{+\infty} \, dy \, y' \int_{-\infty}^{+\infty} \, dz \, e^{-iqz} |\phi_e(x,y)|^2 |\phi_h(x',y')|^2 \frac{1}{\sqrt{x^2 + (y-y')^2 + (x-x')^2}} \]

\[ = 2\varepsilon_0^2 \int_{-\infty}^{+\infty} \, dx \, dx' \int_{-\infty}^{+\infty} \, dy \, dy' |\phi_e(x,y)|^2 |\phi_h(x',y')|^2 . \]

where \( \phi_e(x,y) \) is the quantum wire confinement wave function for the lowest eigenstates of electrons or holes. The exact form of these eigenfunctions depends on the geometry and details of confinement. In the one-loop GW (single particle Green Function (G) and the screened interaction \((W)\)) approximation with dynamically screened interaction, one has [8,32]:

\[ \sum_i (k,z) = -\frac{1}{\beta} \sum_{k',z'} V_s(k-k',z-z') G_i(k',z') \]

\[ = -\frac{1}{\beta} \sum_{k',z'} \left[ e(k-k',z-z') G_i(k',z') \right], \]

where

\[ G_i(k,z) = \frac{1}{z - \varepsilon_{i,k} - \varepsilon_{i,h} - \Delta_i(k) + \mu_i}, \]

and \( \sum e/\hbar(k,z) \) is the self-energy of electrons/holes defined in GW approximation. Also \( \varepsilon_{e,h,k} \equiv \frac{k^2}{2m_e} + E_g^0 \) and \( \varepsilon_{h,k} \equiv \frac{k^2}{2m_h} \) are the bare energies of electron and hole in their respective bands and \( \mu_i \) is the chemical potential. To avoid multi-pole structure in \( G_i(k,z) \), we approximate \( \sum_i(k,z) \) by the momentum-dependent bandgap renormalization \( \Delta_i(k) \). Using the approximation \( \Delta_i(k) \approx \sum_i k^2 (\varepsilon_{i,k} - \mu_i) \), we find the following single pole electron-hole Green's function [8,32]:

\[ G_i(k,z) \approx \frac{1}{z - \varepsilon_{i,k} - \Delta_i(k) + \mu_i}, \]

This is a brief overview of the idea of bandgap renormalization in the dynamical random phase (GW) approximation. After providing the required theoretical background, now we calculate the bandgap renormalization of this quasi-one dimensional systems in the presence of the external electric and magnetic fields focusing on the roles of higher order excitations. Now, we should calculate the screened coulomb potential. Using equation (5), it can be written as:

\[ V_s(k) \]

\[ = 2\varepsilon_0^2 \int \, dx \, dy |\Psi(x,y)|^2 |\Psi(x',y')|^2 . \]

(9)
Using the re-scaled coordinates \( x_i = \frac{x_i}{L} \) and \( x'_i = \frac{x'_i}{L} \), we find:

\[
V_c(k) = \frac{2e^2}{\varepsilon_0} L^2 \int d\bar{x} d\bar{y} \int d\bar{x'} d\bar{y'} |kR| |\Psi(\bar{x}, \bar{y})|^2 |\Psi(\bar{x'}, \bar{y'})|^2,
\]

where \( \bar{\lambda} \) is the re-scaling factor equal to \( 10^{-18}/m^2 \) and \( kR = k \sqrt{(x - x_0)^2 + (y - y_0)^2} \). For simplicity we set \( L = W_e \sim 10 \text{ nm} \). Using \( \Psi(x, y) \) computed numerically in subsection 2.2, we solve the integral of Eq. 9 numerically. Fig. 7 shows the result of this calculation for different values of the relative width of the confinement potential. In this figure, \( V_c(k) \) is normalized by \( \frac{2e^2}{\varepsilon_0} \) and the \( k \) is normalized to \( kL \).

In the next step we calculate the band gap renormalization in the dynamical random phase approximation. To proceed, we need to calculate some quantities numerically. Using the re-scaled quantities \( \bar{k} = kL \) and \( \omega = \bar{\omega} \times 10^{16} \), the single pole Green’s function for electron defined as relation (8) transforms to the following form:

\[
G(k, z) = \frac{1}{1.06 \times 10^{-26} \bar{\omega} - 6.17 \times 10^{-21} \bar{k}^2 L^2 - 2.47 \times 10^{-39} - \Delta_c(k)}
\]

(10)

Also the Green’s function for hole becomes:

\[
G(k, z) = \frac{1}{1.06 \times 10^{-26} \bar{\omega} - 9.2 \times 10^{-22} \bar{k}^2 L^2 + 1.6 \times 10^{-22} - \Delta_h(k)}
\]

(11)

To calculate bandgap renormalization in this configuration, we define the re-scaled \( \beta_e \) and \( \mu_e^0 \) as \( \frac{\beta \hbar^2}{2m_e^2 L^2} = \beta_e \frac{57.5}{L^2} \) and \( \mu_e^0 = \beta_e \), respectively. For simplicity and without loss of generality, we can set \( L = W_e \) where \( W_e \) is the width of the quantum well in the \( x \) direction in nanometer. For holes, we also define the re-scaled \( \beta_h \) and \( \mu_h^0 = \beta_h = \beta_e \left( \frac{m_e}{m_h} \right) \) and \( \mu_h^0 = \mu_e \left( \frac{m_e}{m_h} \right) \), respectively. In all of our computations we assume that the ratio \( \frac{m_h}{m_e} \) is equal to 0.3 and \( m_e \approx 0.067 m_e \). The result of our calculations, using the ground state wave function, for bandgap renormalization in the GW approximation at \( T = 0 \) is shown in Fig. 8. In this figure we have compared the bandgap renormalization in the presence and absence of the external EM fields too. Typical values of the bandgap normalization is \( \sim 10 - 30 \text{ meV} \) depending on the temperature and impurities in the system. Because of consideration of more quantum field theoretical details, dynamical random phase (GW) approximation generally gives results that are more consistent with experiments [10,11]. In fact, generally the dynamical correlation effects tend to
reduce the magnitude of the bandgap renormalization, especially when compared with the quasi-static approximation results, and bring the calculated values closer to the experimental results. Fig. 9 shows that the dynamical random phase GW approximation leads to smaller values of the bandgap renormalization than the quasi static approximation result. This figure is plotted for free-field case.

3. The effects of excited states

The effects of higher order excitations on the bandgap renormalization of quantum wires is an important issue which we investigate here. We study bandgap renormalization in the presence of electric and magnetic fields by considering the first excited state. In the framework of the formalism presented in subsection 2.2 the charge carriers distribution in this excited state with different configurations of the external fields are calculated as given in Figs. 3-6 for different fields configurations. Now we calculate the bandgap renormalization in the GW approximation by incorporating the effects of the first excited state using the formalism presented in subsection 2.3. Fig. 10 shows the result of this calculation in the absence of the external EM fields (solid curve) and in the presence of the external field (open circles). It can be seen that, application of the external EM field leads to more renormalization of the fundamental gap by incorporation of the excited states.

As another important result, in Fig. 11 we compare two situation: bandgap renormalization by considering only ground state wave function and the values of this renormalization by incorporating the effects of the first excited state. It can be observed that, incorporation of the effects of the first excited state leads to larger values of the bandgap renormalization.

4. Conclusion

In this paper we have studied the effects of higher order excitation on the bandgap renormalization of a H-shaped quantum wire. We considered this problem in the presence of external electric and magnetic fields. We analyzed the problem in the framework of the dynamical random phase approximation within a finite difference numerical approach. We have shown that charge carriers distribution in this quasi-one dimensional structure is a sensitive function of an asymmetry parameter $\alpha = W_x/W_y$ which measures the relative width of the wire in two dimensions. Application of the external electric and magnetic field induces a new degree of asymmetry in the system which changes the distribution of the charge carriers and quantum wire many-body properties. The screened Coulomb potential of the H-shaped external confine-
ment is a sensitive function of the asymmetry parameter but its general behavior under variation of the wave number is the same for other possible geometries of quasi one dimensional systems such as T-shaped and V-shaped systems. The calculated band gap narrowing for the H-shaped confinement potential in the absence of the electric and magnetic fields within the dynamical random phase approximation shows a typical gap narrowing of the order of few meV (~0 - 30 meV). We have extended these calculations to the more general cases with inclusion of the effects of external fields and higher order excitations. As an important result, the bandgap renormalization increases with decreasing the wire width as a possible realization of the geometry change. We note that the dynamical random phase approximation leads to smaller values of the bandgap renormalization and more reliable result than quasi-static approximation in comparison with experiments. Application of the external electric and magnetic fields on the quantum wire structure leads to larger renormalization in GW (solid curve) and quasi-static (open circles) approximations in the absence of the external fields.

Fig. 9. Comparison of the values of the bandgap renormalization in GW (solid curve) and quasi-static (open circles) approximations in the absence of the external electromagnetic fields.

Fig. 10. Bandgap renormalization in GW approximation by incorporation of the effects of the first excited state for \( E = B = 0 \) (solid curve) and \( E \neq 0 \) and \( B \neq 0 \) (open circles).

References